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Debye frequency and interplay of superconductivity and antiferromagnetism in high T_c superconductors

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stract . The interplay between superconductivity (SC) and antiferromagnetism (AFM) is studied in strongly correlated systems $R_{2-x}M_x CuO_4$ =Nd, La, Pr, Gd, M=Sr, Ce) due to electron-phonon interaction. It is assumed that SC arises due to BCS pairing mechanism in presence of AFM in lattices of Cu-O planes Debye frequency ω_D dependence of high temperature SC gap as well as staggered magnetic field at different temperatures calculated analytically and solved self-consistently with respect to half-filled band situation for different model parameters (temperature parameter and hybridization parameter v, λ_1 and λ_2 being the SC and AF coupling parameters, respectively). The SC gap and AFM gap are studied in their xistence phase for different Debye frequencies

ywords : Debye frequency, superconductivity, antiferromagnetic gap

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ntroduction

ter Bednorz and Muller [1] discovered high Tc perconductors, there has been great interest in understanding true mechanism responsible for superconductivity in these tems. The scanning tunneling spectroscopic data for Bi/ 12 [2] give the temperature dependence of the SC gap $\Delta(T)$ zero K temperature with $2\Delta(0)/k_B T_c = 7$ to 9. The temperature pendence of the gap of $BI_2Sr_2\ CuO_4$ / $Bi_2Sr_2CaCu_2O_8$ mpound [3] is similar to that of weak coupling in BCS theory, hough the ratio $2\Delta(0)/k_B T_c = 5.8$ significantly exceeds the nventional value 3.5. The point contact spectroscopy for *Bi* / $n-1)n$ [4] suggests that phonons play a dominant role in the perconducting pairing in the compounds with a strong upling with the value of $2\Delta(0)/k_B T_c = 6$ to 8. The phonon structure of the I-V characteristics was also observed in the compounds: LSCO and $EuBa_2Cu_2O_7$ at large values of $2\Delta(0)/k_B T_c = 10$ [5], in Nd – Ce – CuO at $2\Delta(0)/k_B T_c = 3.8$ [6]. Computation of the Eliashberg function, suggests that phonons contribute significantly to the superconducting pairing.

The observation of oxygen-isotope effect strongly indicates that the electron-phonon coupling does contribute to the pairing within all the oxide superconductors. In conventional superconductors, the observation of the isotope effect *i.e.* $T_c \,\alpha\, M^{-\alpha}$ with coefficient $\alpha \simeq 0.5$ was the direct proof of the existence of electron-phonon pairing. The first measurement of α in copper-oxide superconductors revealed a slight change in transition temperature T_c and gave $\alpha \leq 0.2$ in LSCO compounds and $\alpha \leq 0.16$ in YBCO and in the Bi- and Tl- based compounds. Later, a strong dependence of α on the composition was found: the index α increased with the suppression of T_c. Thus, in $La_{2-x}Sr_xCuO_4$, a value $\alpha \simeq 0.6$ was obtained for $x = 0.11$ and $T_c \simeq 30K$; in $Y_{1-x}Pr_x\,Ba_2Cu_3O_7$, a value $\alpha \simeq 0.4$ was observed. The isotope effect is small in the optimized compounds with the maximum T_c *i.e.* in $Nd_{2-x}Ce_xCuO_4$ with electron type conductivity [7]. Thus, the electron-phonon interaction contributes to the superconducting pairing $(\alpha \neq 0)$,

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though its role is not decisive ($\alpha << 0.5$) [8]. In BCS formalism, the superconducting coupling constant λ is related to the phonon energy ω_D (Debye cut-off) near the Fermi surface and is given by $\lambda = N(0)g^2/\left(M\omega_D^2\right)$ with g and $N(0)$ being the average electron-phonon coupling and the density of state at the Fermi surface, respectively. For weak coupling limit in BCS theory, the Debye temperature Θ_D ranges from 100K to 500K in conventional superconductors. The Θ_D for high temperature superconductors is found to be $\Theta_D \approx$ 358K for LSCO, 552K for $Y(Ba,Sr)Cu_3O_7$ and 582K for $YBa_2Cu_3O_{7-y}$ and 695K for $Tl_2Ba_2CaCu_2O_8$.

Antiferromagnetic (AF) spin fluctuations are vitally important in explaining many of the anomalous properties of high temperature superconductors (HTSC)in the normal state. The AF spin fluctuation theory [9] leads to attraction in the d-wave channel in the strong coupling limit, $U>>t$, although under certain assumptions, it can lead to an attraction in the s-channel. A model calculation *via* spin fluctuations in heavy fermion systems by Miyake *et al* [10], indicates the probability of an-isotropic s-wave pairing. On the other hand, pairing mechanisms, based on electron-phonon interaction, polarons *etc.*, would be compatible with pure d-wave, pure s-wave or an admixture of the two [11]. The tunneling experiment done by Sun and Dynes [12] tends to rule out d-wave gap anisotropy Some theoreticians have considered inter-layer tunneling mechanism and extended s-wave gap anisotropy [13] to explain the observed magnitude of the high transition temperature. The high T_c arises due to the tunneling of the Cooper pairs, which are formed in the CuO_2 plane due to phonon- mediation. There have been attempts by Igarashi and coworkers [14, 15] to explain the phenomenon of interplay between superconductivity and antiferromagnetism in cuprate superconductors. The common feature of all these models is the assumption that the large specific heat coefficient arises from the interaction of the strongly correlated electrons in the Cu-O plane with the Nd spins. In these models, the influence of Nd - Nd exchange interaction is neglected. Rout *et al* have used the Fulde model and incorporated the electron-phonon interaction to investigate the velocity of sound [16], Raman spectra [17] and phonon anomaly in high temperature superconductors [18]. Recently, they have reported the interplay of superconductivity and antiferromagnetism in presence of hybridization between conduction and f-electrons in high T_c superconductors [19]. In the above model, we have considered the weak correlation giving rise to antiferromagnetism in the copper oxide plane. Again BCS Type phonon mediated Cooper pairing is considered in the weak coupling limit. Both antiferromagnetism (AFM) and superconductivity (SC) are considered in the mean field approximation.

In the present communication, we incorporate the phonon mediated B.C.S. type Cooper pairing and study the effect of Debye energy on the co-existence of superconductivity and antiferromagnetism. In the introduction, we have reviewed the experimental observations of the magnetic and superconducting properties of the rare-earth cuprates with special emphasis on doped Nd-cuprate. We reviewed the experimental evidence of the role played by phonons and overviewed some theoretical calculations. In Section 2, we describe the theoretical model including B.C.S.-type of pairing mechanism for superconductivity. In Section 3, we calculate the expression for the superconducting gap and staggered magnetic field. In Section 4, we discuss the results.

2. Model Hamiltonian

In the absence of holes in La-based and of electrons in Nd based high T_c systems, the antiferromagnetic exchange usually leads to the Neel ground state which is characterized by a long range antiferromagnetic (AFM) order in the spin alignment of Cu lattice sites. Hence, the copper lattice is divided into two sub-lattices 1 and 2.

The Hamiltonian involving hopping of copper d electron between two adjacent sites is written as

$$H_d = \Sigma_{k\sigma}\,\varepsilon_a(k)\left(a_{k\sigma}^{\dagger}\, b_{k,\sigma} + h.c.\right).$$

Here, $a_{k\sigma}^{\dagger}$ and $b_{k\sigma}^{\dagger}$ are creation operators of electrons at sites 1 and 2 of copper, respectively. The hopping takes place between neighbouring sites of copper with dispersion $\varepsilon_0(k) = 2t(\cos k_x + \cos k_y)$. The antiferromagnetism due to copper lattice can be represented by Heisenberg exchange interaction. However, we introduce a staggered magnetic field of strength h which stimulates strong AFM correlation of copper d-electrons. This can be written as

$$H_s = (h/2)\,\Sigma_{k\sigma}\,\sigma\left(a_{k\sigma}^{\dagger}\, a_{k,\sigma} - b_{k,\sigma}^{\dagger}\, ba_{k,\sigma}\right).$$

When the material is doped, the charge carriers enter the CuO_2 plane and destroys the long range AFM order. Depending on the concentration of the doping and the temperature range, a complex disordered phase is formed in the CuO_2 plane This disorder phase can be represented by the on-site f-level energy of the non-magnetic impurity rare-earth ion (Ce) in NCCO and the hybridization between f-level and the Cu – $3d$ electron band For sufficiently low doping *i.e.* x much less than 0.02, a long range AFM order exists. For a doping concentration of $x =$ 0.058, a long range AFM order yields a short range AFM order and provides a disordered AFM (termed as spin glass) ground state in two dimensions. This is mostly influenced by the degree of hybridization interaction (V). The Hamiltonian

$$H_v = V\,\Sigma_{k,\sigma}\left(a_{k,\sigma}^{\dagger}\, f_{1,k,\sigma} + b_{k\sigma}^{\dagger}\, f_{2,k,\sigma} + h.c.\right)$$

is the effective hybridization between the *f*-electrons at two sub-lattices of rare-earth and the conduction electrons of copper. The Hamiltonian

$$H_f = \varepsilon_f \sum_{k,\sigma}\left(f^{\dagger}_{1,k,\sigma} + f_{1,k,\sigma} + f^{\dagger}_{2,k,\sigma} f_{1,k,\sigma}\right)$$

is the intra *f*-electron Hamiltonian and ε_f is the renormalized *f*-level energy. Total electronic Fulde Hamiltonian [15] is written

$$H_0 = H_d + H_s + H_v + H_f \,. \tag{1}$$

Here, B.C.S. type of phonon mediated Cooper pairing of conduction electrons of two different copper sites in the Cu-O is taken into account. The super-conducting state of the system is described by the interaction Hamiltonian

$$H_1 = -\Delta \sum_k \left[\left(a^{\dagger}_k\, a^{\dagger}_{-k} + a_{-k}\, a_k\right)z + \left(b^{\dagger}_k\, b^{\dagger}_{-k} + b^{\dagger}_{-k}\, b_k\right)\right], \tag{2}$$

where

$$\Delta_k = -\sum_k \bar{V}_k\left(\left\langle a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\uparrow}\right\rangle + \left\langle b^{\dagger}_{k\uparrow} b^{\dagger}_{-k\uparrow}\right\rangle\right). \tag{3}$$

Here, Δ_k is the superconducting gap parameter and $\bar{V}_k$ is the interaction potential between the pairing electrons. However, we have neglected the inter-site sub-lattice Cooper pairing of the conduction electrons for the simplicity of calculation. The total Hamiltonian is

$$H = H_0 + H_I \,. \tag{4}$$

3. Expression for SC gap and staggered field

We have a limitation on the *k*-sum owing to the restriction that the attractive interaction is only effective with energy $|\varepsilon_1 - \varepsilon_2| < \omega_D$. Here, the attractive interactions between two carriers are ε_1 and ε_2 to form the Cooper pair and ω_D is the Debye frequency. Further, we adopt the following simplified form for the interaction potential $\bar{V}_k$ in the ordinary isotropic weak coupling limit. Here, $\bar{V}_k = -V_0$, if $|\varepsilon_1 - \varepsilon_2| < \omega_D$; $\bar{V}_k = 0$, otherwise. In this approximation, we assume that the gap parameter is independent of *k*. The final expression for superconducting energy gap is

$$\Delta(T) = V_0 N(0) \int^{\omega_D} d\varepsilon_0(k)\left[F_1(k,T) + F_2(k,T)\right], \tag{5}$$

where

$$F_1(k,T) = \frac{(\Delta - h/2)}{2\sqrt{E^4_{1k} - 4V^4}}$$

$$\left[\omega_1(k)\tan h\left(\frac{1}{2}\beta\omega_1\right) - \omega_2(k)\tan h\left(\frac{1}{2}\beta\omega_2\right)\right]$$

and

$$F_2(k,T) = \frac{(\Delta + h/2)}{2\sqrt{E^4_{2k} - 4V^4}}$$

$$\left[\omega_3(k)\tan h\left(\frac{1}{2}\beta\omega_3\right) - \omega_4(k)\tan h\left(\frac{1}{2}\beta\omega_4\right)\right]. \tag{6}$$

The staggered magnetic field h is given by

$$h = -\frac{1}{2} g\mu_B \sum_{k,\sigma}\left[\left\langle a^{\dagger}_{k,\sigma} a_{k,\sigma}\right\rangle - \left\langle b^{\dagger}_{k,\sigma} b_{k,\sigma}\right\rangle\right], \tag{7}$$

where g and μ_B are Lande *g*-factor and Bohr magneton, respectively. The correlation functions

$\left\langle a^{\dagger}_{k,\uparrow} a_{k,\uparrow}\right\rangle, \left\langle a^{\dagger}_{k,\downarrow} a_{k,\downarrow}\right\rangle, \left\langle b^{\dagger}_{k,\uparrow} b_{k,\uparrow}\right\rangle$, and $\left\langle b^{\dagger}_{k,\downarrow} b_{k,\downarrow}\right\rangle$ are calculated. The final expression for the staggered magnetic field is

$$h = -\frac{1}{2} g\mu_B N(0) \int_{+W/2}^{-W/2} d\varepsilon_0(k)\left[F_1(k,T) - F_2(k,T)\right], \tag{8}$$

where $F_1(k, T)$ and $F_2(k, T)$ are defined in eq (6). We put $\sum_k \rightarrow \int N(0) d\varepsilon_0(k)$ with integration limit $-W/2$ to $+W/2$ where $N(0)$ is the density of states of the conduction electrons at the Fermi level ε_F.

Different physical parameters are made dimensionless by dividing them by $2t$ where $W = 8t$ is the width of the conduction band. They are

$$\frac{\Delta(T)}{2t} = z;\ \frac{\omega_D}{2t} = \tilde{\omega}_D;\ \frac{k_B T}{2t} = \theta;$$

$$\frac{h}{2t} = h;\ \frac{V}{2t} = V;\ \frac{\varepsilon_0(k)}{2t} = x_0\,;$$

$$N(0)V_0 = \lambda_1;\ \lambda_2 = N(0)_{g\mu_B}/2\,. \tag{9}$$

4. Results and discussion

We solve equations for Δ and h numerically and self-consistently. Different dimensionless parameters involved in the numerical calculation are the superconducting coupling λ_1, antiferromagnetic coupling λ_2, superconducting gap z, staggered magnetic field h, hybridization strength V, and temperature parameter $\theta = k_B T/2t$. Here the Fermi level (ε_F) is taken to be 0, *i.e.* lying at the middle of the conduction band.

The f-level ε_f coincides with the Fermi level. A standard set of parameters are chosen as follows: $\lambda_1 \sim 0.15$, $\lambda_2 \sim 0.185$, $V \sim 0.003$ and the conduction band width $W \sim 1ev$. The parameter λ_1 is smaller than the maximum value of SC coupling ($\lambda_1 \simeq 0.33$), observed in conventional BCS type phonon mediated superconductivity. This observed low value of SC coupling agrees with the experimental observations.

The SC gap (z) and AFM gap (h) are solved self-consistently and their temperature dependence is shown in Figure 1. The effect of two Debye frequencies $\tilde{\omega}_D = 0.31$ and 0.33 on the gaps are considered, because they correspond to the critical temperature $\theta_c \simeq 0.01$ (*i.e.* $T_c \simeq 25K$) for Nd_2–Ce–CuO system. It is observed in Figure 1 that the SC gap near absolute zero is not affected at all. However, the increase of Debye frequency suppresses the SC gap and transition temperature in high-T_c superconductors, which contradicts the BCS prediction for conventional superconductors. Moreover, the SC transition at T_c is not sharp. The effect of Debye energy on the staggered magnetic field is not well known both theoretically and experimentally. Figure 1 shows the variation of AFM(h) with temperature for different Debye frequencies. The increase of Debye energy enhances the staggered field throughout the temperature range as well as Neel temperature. However, this behaviour of AFM gap due to the phonon energy is not expected. Hence, the AFM gap exhibits anomalous behaviour.This arises due to the interplay of AFM and SC.

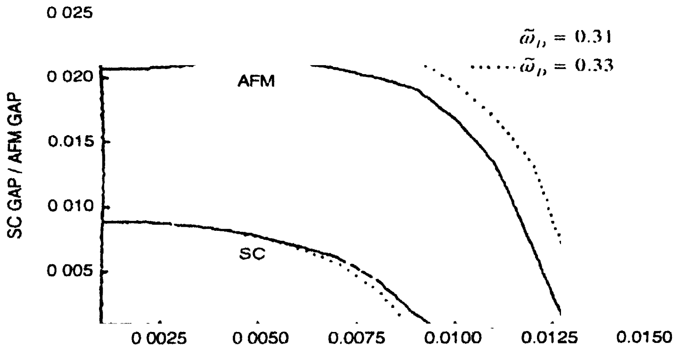

Figure 1. The plot of SC GAP (z) / AFM GAP (h) *vs* O for two different values of Debye frequency $\tilde{\omega}_D$ = 0.31, 0.33 for fixed value of λ_1 = 0.15, λ_2 = 0.003.

The variations of the AFM gap (h) and SC gap(z)with the Debye frequency for two different temperatures θ =0.004 and 0.006 are shown in Figure 2. The AFM gap increases almost linearly with the increase of the Debye frequency. The AFM long range order is expected to increase with the spin ordering. But it should be independent of Debye energy in its independent state in absence of superconductivity. However, the AFM order increases with Debye energy as shown in Figure 2. This is possible due to interplay of AFM and SC. Hence, the phonon energy plays a vital role in high-T_c cuprates. Figure 2 shows the general trend of AFM and SC gap over a large Debye frequency range 0.25 ($\simeq$ 625 K) to 0.33 ($\simeq$ 775 K). For Debye frequency $\tilde{\omega}_D < 0.25$, the SC gap is not stabilized. Hence, the minimum phonon energy required to form Cooper pairs is of the order of $\tilde{\omega}_D = 0.25$ ($\simeq$ 625 K). For phonon energy $0.25 \le \tilde{\omega}_D \le 0.29$, the SC gap remains almost constant. Hence, the Cooper pairing is independent of the increase of Debye frequency. Again, the Cooper pairing is suddenly enhanced for phonon frequency from 0.29 to 0.30 and attains a maximum value for $\tilde{\omega}_D$ =0.30 The enhancement of the SC gap in this range of Debye frequency is accompanied by corresponding small enhancement in AFM gap as shown in Figure 2. On further increasing the Debye frequency, the superconductivity instead of increasing starts decreasing slowly. It means that it causes a very small pair breaking of the Cooper pairs but enhances the AFM order. When the temperature is decreased from θ = 0.006 to 0.004, the z vs. ω_D graph retains its nature accompanied by the enhancement of the SC gap.

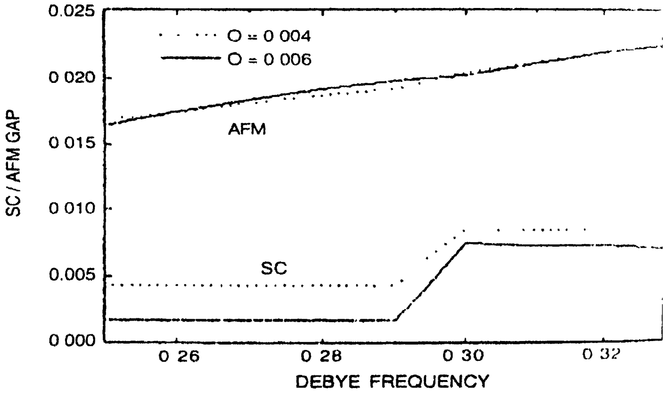

Figure 2. The plot of SC GAP (z) / AFM GAP (h) *vs* Debye frequency for two temperatures θ = 0.004, 0.006 for fixed values of λ_1 = 0.15, λ_2 = 0.185 and V = 0.003.

The influence of Debye frequency $\tilde{\omega}_D$ on the coexistence of AFM and SC phase is explained below. A uniform SC order exists for $0.25 < \tilde{\omega}_D < 0.29$ due to the phonon mediated intra-site Cooper pairing of the type $\langle a^{\dagger}_{k\downarrow} a^{\dagger}_{-k\downarrow} \rangle$ and $\langle b^{\dagger}_{k\uparrow} b^{\dagger}_{-k\downarrow} \rangle$ corresponding to two different Cooper sites. But the induced inter-site Cooper pairing of the types $\langle a^{\dagger}_{k\downarrow} a^{\dagger}_{-k\downarrow} \rangle$ and $\langle b^{\dagger}_{k\uparrow} b^{\dagger}_{-k\downarrow} \rangle$ enhances the SC order within a range of Debye frequency *i.e.*, $0.29 \le \tilde{\omega}_D < 0.30$. The small enhancement of the AFM order within this range of $\tilde{\omega}_D$ may be due to the presence of a small antiferromagnetism induced in the impurity f-electron states. The superconductivity attains an optimum value for $\tilde{\omega}_D \simeq 0.30$. For $\tilde{\omega}_D \simeq 0.30$, one observes the pairing breaking effect in the

SC phase and consequently, the slow decrease in the SC order. This SC pair breaking is accompanied by an enhancement of the AFM order. The range of Debye temperature discussed in this model calculation is of the same value *i.e.*, $\tilde{\omega}_D$ = 358 K to 695 K observed in different high - T_c systems. Hence, the effect of Debye frequency on the interplay of the SC and AFM phases appears to be reasonable on the basis of the present model calculation.

In Figure 3, we study the effect of Debye frequency on the SC gap (z) in absence of antimagnetism. The variation z *vs.* $\tilde{\omega}_D$ is plotted for the values of λ_1 = 0.15, V = 0.003 and θ = 0.006 as of Figure 2. The SC gap increases linearly up to $\tilde{\omega}_D \simeq$ 0.2 and again increases linearly beyond $\tilde{\omega}_D > 0.2$ with slightly decreasing slope. This shows similar variation in transition temperature T_c with Debye energy $\tilde{\omega}_D$ for a fixed value of coupling constant λ_1. The T_c variation in BCS model is given by $kT_c \simeq \hbar\omega_D \exp(-1/\lambda_1)$. However, the SC gap ($z$) variation with Debye frequency shows linear dependence only in a narrow range of $0.29 < \tilde{\omega}_D < 0.30$ in the coexistence phase as shown in Figure 2. Figure 4 shows the effect of hybridization between f-level and conduction electron on SC gap and AFM gap. The SC gap remains unaffected with increase of hybridization for low values of $\tilde{\omega}_D$ (0.24–0.29) in this range, the Cooper pairing is so strong that the hybridization cannot cause pair breaking. The SC gap is suppressed with increase of hybridization for $0.29 \geq \tilde{\omega}_D < 0.30$, the suppression being higher, for higher $\tilde{\omega}_D$ value. Further, for the still higher range of $\tilde{\omega}_D$ (0.30–0.33), this trend becomes more pronounced. The effect of hybridization between the conduction band and f-electron level on the AFM gap is shown in Figure 4(upper plot). As the hybridization increases from V=0.003 to 0.005, the AFM gap is suppressed throughout the temperature range.

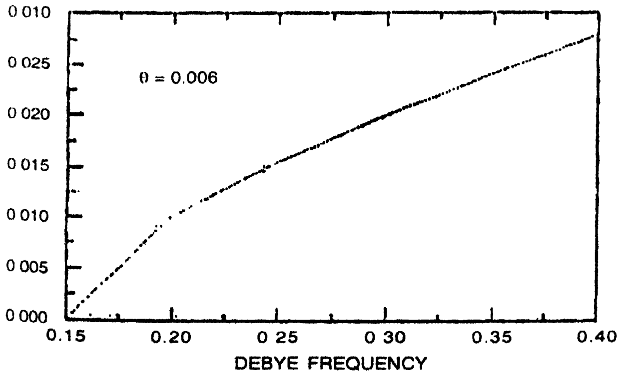

Figure 3. The plot of SC GAP(z) *vs.* Debye frequency for temperature 0.006, λ_1 = 0.15 and V = 0.003

It is observed that both the SC and the AFM long range order are suppressed with the increase of hybridization between f-electron and conduction electron. This suppression can be explained on the basis of the Cooper pairing amplitude like $\phi^C = \langle a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}\rangle$ and $\langle b^\dagger_{k\uparrow} b^\dagger_{-k\downarrow}\rangle$, mixed pairing amplitudes $\phi^M = \langle a^\dagger_{k\uparrow} f^\dagger_{-k\downarrow}\rangle$ and $\langle b^\dagger_{k\uparrow} f^\dagger_{-k\downarrow}\rangle$, and only f-electron pairing amplitudes $\phi^F = \langle f^\dagger_{k\uparrow} f^\dagger_{-k\downarrow}\rangle$ and the hybridization amplitudes and $\phi^V = \langle a^\dagger_{k\sigma} f_{-k\sigma}\rangle$ and $\langle b^\dagger_{k\sigma} f_{-k\sigma}\rangle$. The Cooper pairing was present originally in a-site and b-site of the lattice in the form of the amplitude ϕ^C. When the conduction electron and f-electrons are hybridized, there occurs pair breaking in amplitudes ϕ^C. Induced SC pairing occurs due to the formation of the pairing amplitudes like ϕ^M, ϕ^F and the hybridization amplitude ϕ^V. This results in the suppression of SC order parameter with increase of the hybridization strength. The exact nature of the suppression of SC gap can be studied by the temperature dependence of the amplitudes like ϕ^C, ϕ^M, ϕ^F and ϕ^V.

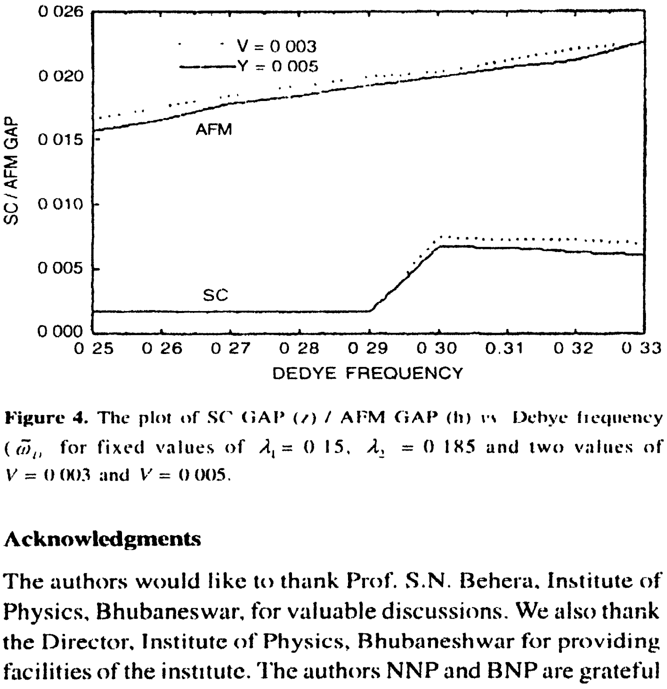

Figure 4. The plot of SC GAP (z) / AFM GAP (h) *vs.* Debye frequency ($\tilde{\omega}_D$ for fixed values of λ_1 = 0.15, λ_2 = 0.185 and two values of V = 0.003 and V = 0.005.

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